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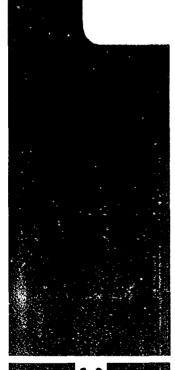
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REMEDIATION TECHNOLOGIES INC

GROUNDWATER MODELING AT THE BURLINGTON NORTHERN SITE SOMERS, MONTANA

Prepared for Glacier Park Company

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Prepared by Remediation Technologies, Inc.

September 1988

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TABLE OF CONTENTS

1.0	INTRODUCTION	1
2.0	SITE DESCRIPTION	3
	2.1 Geologic Setting	3
	2.2 Field Data	8
3.0	ANALYTICAL MODEL	10
	3.1 Description of Model	10
	3.2 Assumptions	10
	3.3 Data Input	15
	3.4 Parameter Values	17
	3.4.1 X-Coordinate Values	19
	3.4.2 Y-Coordinate Values	19
	3.4.3 Time Steps	19
	3.4.4 Velocity, Hydraulic Conductivity, and	
	Gradient	20
	3.4.5 Longitudinal Dispersi n Term	21
	3.4.6 Transverse Dispersion Term	22
	3.4.6 Transverse Dispersion Term	
	3.4.7 Half Length of Strip Source	22
	3.4.8 Decay Factor of Solute	23
	3.4.9 Retardation Factor	23
	3.4.10 Decay Factor of the Source	25
	3.4.11 Initial Concentration of Solute in	
	Groundwater	25
	3.4.12 Summary of Model Parameters	26
4.0	MODELING RESULTS	33
	4.1 Model Calibration	3:
	4.2 Sensitivity to Hydraulic Conductivity	4:
	4.3 Sensitivity to Dispersivity	4:
	4.4 Sensitivity to Biodegradation of the Solute	4:
	4.5 Hypothetical Source Removal	5
5.0	SUMMARY AND CONCLUSIONS	59
6.0	REFERENCES	6
A DDEN	NDTY X	61

1.4

13

15#

LIST OF FIGURES

<u>Figure</u>

2-1	Boring Log of Well #88-1	4
2-2	Boring Log of Well #88-2	5
2-3	Boring Log of Well #88-3	7
3-1	Two-Dimensional Plane Dispersion Model	11
	Predicted Transport of Naphthalene based on Actual Field	
• -	Measured Values	34
4-2	Measured Values	35
4-3	Results of Model Run #25	36
1-1	Plume Map based on Run #25	37
4-5		3 /
4-5	Details of Coefficients	39
	Retardation Coefficients	
	Transport of Naphthalene with No Retardation	40
4-7	Comparison of Naphthalene Transport Distances with	
	Varying Hydraulic Conductivities	42
	Plume Map	44
	Plume Map	45
4-10	Plume Map	46
	Plume Map	47
4-12	? Comparison of Naphthalene Transport Distances with	
	Differing Initial Concentrations and Retardations	48
4-13	Comparison of Naphthalene Transport Distances with	
	Differing Initial Concentrations and Retardations	49
4-14	Comparison of Naphthalene Transport Distances with	
	Differing Dispersivities	50
4-15		
	Differing Dispersivities	51
4-16		
	Aerobic and Denitrification Degradation	53
4-17		٠.
7 4,	Times under Denitrification Conditions	54
4-18		J.,
4-10	Times with a Half-Life of 1 Year	56
4 10	O Comparison of Naphthalene Transport Distances with	50
4-15	Half-Lives of 2 and 3 Years	56
		50
4-2(Naphthalene Transport Distances after 60 years Assuming	
	Source Removal down to the 1 ppm Level	58

LIST OF TABLES

Tabl	<u>e</u>							
	Hydraulic Conductivities							9
	and Cleary and Ungs Analytical Solution .	•						12
3-2	Verification of Analytical Code							18
3-3	Input Parameters for Runs #1 through #6 .	•						27
	Input Parameter for Runs #7 through #12 .							28
3-5	Input Parameters for Runs #13 through #18							29
3-6	Input Parameters for Runs #19 through #2							30
3-7	Input Parameters for Runs #25 through #30							31
3-8	Input Parameters for Runs #31 through #34	•	•	•	•	•	•	32

1.0 INTRODUCTION

The Work Plan for Additional Investigations at the Somers Tie Plant provided an outline of activities to be conducted for hydrogeologic investigations and computer modeling in response to comments received for the Remedial Investigation Report (ReTeC, 1987a), the Feasibility Study (ReTeC, 1987b), and the Risk Assessment Report (ReTeC, 1987c). The modeling effort was proposed to refine the current understanding of existing site conditions and to project future groundwater quality conditions under various scenarios at the Somers site.

In March 1988, several initial analytical model runs were conducted to determine the feasibility of proceeding with a numerical model and to determine the extent of additional field work (ReTeC, 1988). As a result of these model runs, it was decided to install three new groundwater monitoring wells downgradient from the CERCLA Lagoon. These three new wells were subsequently sampled along with two other wells in the vicinity of the CERCLA Lagoon. The results of this sampling event have been used to calibrate the modeling efforts and have been incorporated into this report.

The transport of naphthalene as a solute down-gradient from the CERCLA Lagoon area was modeled with a two-dimensional analytical solution to the advection-dispersion equation. The transport of naphthalene was modeled because it has the highest mobility in water compared to the other polynuclear aromatic hydrocarbons present at this site. Modeling naphthalene transport will therefore account for the greatest extent of plume migration. The delineation of the maximum extent of the downgradient plume from the Cercla Lagoon is the primary concern of this modeling effort.

133

The modeling effort included the results of the most recent groundwater sampling event conducted in June 1988. In all, 34 model runs were conducted. Section 2.0 presents the site

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description including a synopsis of the geology and the acquisition of the field data. Section 3.0 presents the details on the analytical modeling including the area modeled, the parameters used to run the model, and the variations of these parameters. The modeling results are presented in Section 4.0 and the summary is included in Section 5.0.

2.0 SITE DESCRIPTION

2.1 Geologic Setting

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The geologic setting of the Somers site was documented in the Remedial Investigation (ReTeC, 1987a). The RI shows the area of the Cercla Lagoon to consist of interbedded silts, clays, and fine-grained sands deposited in a deltaic environment. A small prograding delta formed in areas where the Flathead River entered Flathead Lake. The site of this delta would change through time as the Flathead River meandered across the valley. In areas abandoned by the river as it changed its course, sediment influx would be diminished causing the previously deposited sediments to be reworked by the action of the lake.

The Flathead River at one time entered Flathead Lake in the vicinity of the Somers site, as evidenced by the slough which is a cut-off meander loop of the river. The subsurface geology of the CERCLA Lagoon area consists mainly of silts and clays with minor interbeds of fine-grained sands. These lithologies are interpreted to have been formed as either distal portions of over-bank deposits and crevasse splays or as prodelta muds prograding into the lake.

Figures 2-1, 2-2, and 2-3 present the boring logs of the three new wells installed in June 1988. The logs document the generally fine-grained nature of the sediments and show a general progression of clayey silt to very-fine sand grading with depth into clay with interbeds of medium-grained sand. Analysis of split spoon samples in the field indicated that a three to four foot sand bed in the clay unit was the cleanest, best sorted, coarsest grained, and most permeable unit encountered. This unit is referred to as the deltaic sand aquifer in this report. It was felt that monitoring the deltaic sand aquifer would give the worst case results because any contaminant would be able to migrate furthest through this permeable unit.

RET	EC	R I	-	OGIES			OG BORING SOME 1				
PROJECT	Somers				СО	NTRACTOR Hillman Drilling	MONUMENT				
PROJECT *		11-320			DR	ILLER Ed Hillman/Joe Berry	RISER 2" PVC Sch. 40 Flush Joint				
LOCATION	near CE	RCLA lag	000		RIG	TYPE Schram Rotodrill	SCREEN 2" PVC** 27' to 37'				
TOTAL DEPT	ዝ 37	7'			ME	THOD hollow stem auger*	FILTER PACK *** 23' to 37'				
DATE .M	1ay 11,	1988			CA	SING ID 4 1/4"	SEAL **** 20'2" to 23'				
STARTED	5-11 (OMPLETE	D.	5-13	ВО	RING ID 6 7/8"	GROUT				
LOGGED BY	AMC				BIT	TYPE GROUND ELEV					
SAMPLE TYPE AND NUMBER	BLOWS Per 6 in.	DEPTH RANGE	% REC	рертн FT.	•	SAMPLE DESCRIPTION CLASSIFICATION SCHEME_					
modified split spoon split spoon	paldues paldues paldues	10-12 12-14 15-17 17-19 19-21 21-23 23-25 25-27 27-29 29-31 33-35 37-39	18" 3" 24" 24" 24" 24" 24" 24" 24"	- 5 - 10 - 15 - 20 - 25 - 30 - 35 - 40		spots, orange mottling chronecovered 1' 12-14 Same as above with finer material at 12', very 15-17 Silty, gray, some verous creo nodules, clumps 17-19 Silt, gray, some verends), brown creo nodules - 19-21 Clay, gray, moist, recomposed Clay, gray, gray	air drilling rotary moist n, creosote odor, staining, oily in ughout pushed spoon 5-10'; orange mottling throughout, saturated, fine sand, silty, creosote odor, visible oil ery fine sand, very moist, oily, surrounding vegetal matter ry fine sand (more in center than at first foot then none below no creo visible but odor present no creo visible but odor present limed grained-3"; clay-2", sand-6" med grained, saturated throughout lightly coarser grained sand or, moist ry slight odor				
GROUNDWA1	TER DEPT	H(FT)				DATE/TIME					
REMARKS:		r 10 feet					Sand				
Attempted Attempted	d Shelby		no	recove	ry		lected were analyzed for PAH, ZN				

Figure 2-1

RBT	EÇ-		_	OGIES			7						
PROJECT	Somers	MT			CO	ONTRACTOR Hillman Drilling MONUMENT	1						
PROJECT *		11-320				RILLER Ed Hillman/Joe Berry RISER	ᅦ						
LOCATION			LA lag	oon		G TYPE Schram Rotodrill SCREEN 2" PVC** 28' to 38'	٦						
TOTAL DEPT					ME	THOD hollow stem auger* FILTER PACK *** 20' to 21'.6"	_						
DATE 1	1ay 12,	1988			CA	ASING ID 4 1/4" SEAL **** 19' to 20'	_						
STARTED	5-12 (COMPLETE	D	5-12	80	DRING ID 6 7/8" GROUT							
LOGGED BY	AMC	;			ВІТ	T TYPE GROUND ELEV							
SAMPLE TYPE AND NUMBER	BLOWS Per 6 in.	DEPTH RANGE	8 8	ре тн FT.		SAMPLE DESCRIPTION USCS CLASSIFICATION SCHEME.							
Split spoon 1 2 3 4 5 6	poldues poldues	5-7' 7-9' 9-11' 11-13' 13-15' 15-17'	24"	5 ST CL ST CL 10	- - - -	5-7 Sand, gray, orange mottling, very fine/clay, gray, slightly sandy, creosote nodules, odor, follows root zones, moist, 2 zones each several inches thick, slightly silty 7-9 Sand, gray, orange mottling, very fine/clay, gray, slightly sandy, creosote nodules odor, follows root zones, moist, 2 zones each several inches thick, slightly silty 9-11 Sand, gray, silty, orange mottling, fine sand 5", rest is clay, gray, CL, large creo stain in sand zone, moist, slightly silty 11-13 Clay, slightly silty, sand & odor has decreased, no visible evidence of creo, one end slightly greater sand content, moist 13-15 Clay, silty, slightly sandy, very slight smell, gray 15-17 Clay, silty, gray, very soggy in 4" (4" from top) rest is moist, no fines, no odor							
8 9		19-21' 21-23'	1	- 20)	19-21 Clay, silty, gray, very moist, soggy at top 21-23 Clay, silty, gray, slightly tighter clay	-						
10	sempled	23-25	24	- 25	;	23-25 Clay, silty, gray, no odor, no sand, moist, soggy at top -							
GROUNDWA	TER DEP	TH(FT)	l	 		DATE/TIME							
REMARKS:	***	America	in Colid	old crur		t *** 10-20 Colorado Silica Sand es .							

Figure 2-2

RETI	EC			I A T OGIES			G BORING \$-68-27 0 € € SHEET 2 OF 2						
PROJECT S	Somers	, MT			CO	NTRACTOR Hillman Drilling	MONUMENT						
PROJECT *	86-0	11-320			DR	ILLER Ed Hillman/Joe Berry	RISER						
LOCATION ac	ross fr	om CERC	LA lag	oon	RIG	RIG TYPE Schram Rotodrill SCREEN 2" PVC** 28' to 38'							
TOTAL DEPTH					ME	METHOD hollow stem auger* FILTER PACK *** 20' to 2							
DATE May	y 12, 1	1988			CA	ASING ID 4 1/4" SEAL **** 19' to 20'							
STARTED 5-	-12 C	OMPLETE	D 5	5-12	80	ORING ID 6 7/8" GROUT							
LOGGED BY	AMC			,	BIT	TYPE	GROUND ELEV						
SAI1PLE TYPE AND NUMBER	BLOWS PER 6 IN.	DEPTH RANGE	338 86	ыртн FT.		SAMPLE DESCRIPTION CLASSIFICATION SCHEME	USCS						
11		25-27 [.] 27-29	24" 24"	- 30	CL .	25-27 Clay, silty, gray, no 27-29 Clay, silty, gray, ind (missed 2' of soll core some	creasing clay content with depth,						
13		31-33	24"			31-33 8" sand, gray, fine grained, 12" clay, silty, gray, no visible evidence of creosote, magic marker odor 33-35 Clay, very sandy, gray, saturated, creo odor							
14	rampled	33-35	24"	-									
15	ŭ	35-37	24	- 35		35-37 Clay, silty, no sand, no odor, wet							
16	sampled	37-39 [.]	24	- 40		37-39 Clay, sandy, wet, very slight magic marker smell in top portion							
				, resp			_						
				_			_						
GROUNDWATE	ם חבחד	שובדי הווידי	l			DATE/TIME							
REMARKS:	* after	r 10 feet America	n Collo	id crur	nble	. *** 10-20 Colorado Silica S	Sand						

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Figure 2-2

ROJECT	SOMERS				CONTRACTOR: GHT	HONUMENT B" / 20" STEEL
FOUECT *	011	-141			DRILLER ERIC BILL	RISER 2" PUC 5CH 40 FLUSH
NOT TROO					BIG TYPE CHE-50	SCREEN 1) 02 OLOT
OTAL DEP	TH 8	2.5'	,,, <u></u>		METHODHOLLOW STEM AUGER	FILTER PACK 10-20 SILICA
HE 6-9	-88				CASINO ID 3.25"	SEAL 8-20 BENTONITE
TARTED	6-9	COMPLET	ED 6	-11	BORING ID 8.0"	GROUT PORTLAND CEMENT
OGGED BA	HOL.	GUEHTH	ER	+ V/A.4.**	BIT TYPE AUGER	GROUND ELEV 2898
SAMPLE TYPE AND WINSER	BLONS PER 6 IN	DEF1H FRNGE	%. 2EC	DEPTH FEET	SAMPLE DESCRIPTION CLASSIFICATION SCHEME	Usca
				- 5	0-14 FEET HL VERY F 10VR 5/3 VERY SLIGHT I	
	,			16		
				- 20 - 25		
T SPO011		ù		- 30	95-38.5 FEET SN SILTY VERY FINE SAME 10YR 4/1 HET MODERATE PLASTICITY	TY VERY FINE SAND (40) TE PLASTICITY
SFL 17	4	35 - 33	CO1	40 45	(20) 5V 5/1 NOIST	(5) VERY FINE SAHDY SILT LON PLASTICITY
				- 50	51 5-50 FEET SM OU. 10YR 471 HET VERW SI	

BENNARS: BORING WAS SEALED WITH BENTONITE FROM \$2.5 TO 53.5 FEET BENTONITE PLUGGED AUGER OF 55 FEET BO AUGER DAS MULLED AUG THE COMPANION RE-DATLLED TO 60 FEET. ODOROUS SILTY SAND DETECTED FROM 52.0 TO 59.5 FEET

2.2 Field Data

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The area modeled in this report consists of approximately a 200 x 1500 ft portion of the Somers site bounded on the upgradient side by the CERCLA Lagoon and extending down-gradient for 1500 feet towards Flathead Lake. Ten monitoring wells have been placed in the vicinity of the CERCLA Lagoon and include Wells #84-12, #84-13, #84-14, #84-16, #85-6a&b, #85-7, #85-8a&b, #88-1, #88-2, and #88-3. Water level measurements, as well as slug tests on some of the wells provided information on the hydrology of this area. In addition, analyses of samples taken in June 1988 from down-gradient Wells #88-1, #88-2, #88-3, #85-6a, and #85-7 provided data with which to calibrate the computer model.

Groundwater flow in the vicinity of the CERCLA Lagoon occurs as essentially linear flow in a east to southeasterly direction towards Flathead Lake with a gradient of 0.010 ft/ft. Water table fluctuations in the vicinity of the CERCLA Lagoon are on the order of about 2 feet in a year. The water level variations in Flathead Lake do not appear to influence the groundwater flow regime in the modeled area.

In order to determine the hydraulic conductivity in the area down-gradient of the CERCLA Lagoon, slug tests were performed on Wells #88-1, #88-2, #88-3 and #85-6a. Each well was tested twice and the results averaged. The hydraulic conductivities of the four wells were all very close in magnitude. Table 2-1 presents the hydraulic conductivities calculated from each of the slug tests. The average hydraulic conductivity of these four wells is 3.25×10^{-3} cm/sec, which for the purposes of modeling was rounded to 3.3×10^{-3} cm/sec.

PROJECT	SOMERS	104			C	CONTRACTOR: GHT MONUMENT 6" X 30" STEEL
PROJECT "	011	-141			D	DRILLER ERIC BALL RISER 2" PUC SCH 40 FLUSH
_OCRTION	******				F	RIG TYPE CHE-50 SCREEN 0 02 SLOT
TOTAL DEP	TH a:	2.5'			11	METHODHOLLON STEM AUGER FILTER PACK 10-20 SILICA
UNIE 6-9	-68				C	CASING ID 3.25" SEAL 6-20 BENTONITE
STARTED	5-9 (OMPLET	ED 15.	-11	В	BORING ID 8.0" GROUT PORTLAND CEMENT
LOGGED BY	NHOL	GUENTH	ER		B	BIT TYPE AUGER GROUND ELEV 2898
SAMPLE TYPE AND HUMBER	BLOWS PER 6 IN	ERPTH RANGE	₩ SEC	DEPTH	•	SAMPLE DESCRIPTION USCS CLASSIFICATION SCHEME
24"X2" SPLiT SPCON	(n	5355.	201	5! 6(53-59.5 FEET SM SILTY MEDIUM SHMD (25) 5Y 5/1 RED/BROWN POORLY SORTED SHMD WITH BLACK ORGANIC FLAKES (3) ROOT CASTS AND WOOD CHIPS WET NON PLASTIC FINES INCREASING WITH DEPTH CREOSOTE ODOR NO VISIBLE STAINING
SHELBY TUBE	(r)	c8 5'-70.5'	50	65 76	Q	59 5-68.5 FEET ML CLAYEY (5) FINE SANDY SILT (15) 59 571 MET SLIGHT PLASTICITY POROUS AND LORMY NO ORGANIC MATERIAL OR ODOR 68.5-70.5 FEET ML CLAYEY (5) FINE SANDY SILT (15) MET SLIGHT PLASTICITY 70.5-80.5 FEET ML CLAYEY SILT LORM (10) IMPEST/I LOMORGHSEODIRMASTICITY
SHELE? TUEE	ч	80.532.5	01	9: 9:	5	80.5-82.5 FEET SILT LOAM SV 5/1 MOIST LOW PLASTICITY BOTTOM OF BORING AT 82 5 FEET
GROUNDHEI	ER DEPT	H(FT)	<u></u>	. 15 - 0	TO	DATE/TIME 5-11-88 1435

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TABLE 2-1 Hydraulic Conductivities

Well Number	Hydraulic Conductivity
S-88-1	3.18 x 10 ⁻³
S-88-2 S-88-2	2.68 x 10 ⁻³ 2.73 x 10 ⁻³
S-88-3 S-88-3	2.35 x 10 ⁻³ 2.42 x 10 ⁻³
S-85-6A S-85-6A	4.6×10^{-3} 4.8×10^{-3}

3.0 ANALYTICAL MODEL

3.1 Description of Model

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The Cleary and Ungs (1978) analytical solution was chosen to simulate flow and naphthalene transport in the CERCLA Lagoon The solution assumes a homogeneous, isotropic, porous medium having unidirectional steady state flow. The two dimensional solution represents the source as a strip rather than a point, thereby more closely representing the actual shape of the CERCLA Lagoon. The aquifer is assumed to be infinite in areal Figure 3-1 presents a schematic diagram of the model extent. which orients the x-axis in the direction of flow. The length of the strip source is equivalent to length 2A along the y-axis. Velocity (V) is the average pore water velocity. presents the analytical equation for the two dimensional strip model including both longitudinal and transverse dispersion. boundary conditions and analytical solution to the equation are also presented in Table 3-1.

This analytical solution was chosen for the Somers site because it represents a relatively simple solution to the advection-dispersion equation, it is easy to use, it is two-dimensional, and it represents the source area as a strip rather than a point, which is applicable to the CERCLA Lagoon at Somers. The solution can also be used as an additional verification to numerical models such as the U.S. Geological Survey (USGS) Solute Transport Model (Konikow and Bredehoeft, 1978).

3.2 Assumptions

Before discussing the various input variables used in the modeling runs and the results of the modeling effort, a review of the assumptions used in the development of this particular model is in order.

1. Darcy's Law is valid. For the Somer's site, this assumption is in all probability correct. The cal-

2a 0070000 SCHEMATIC DIAGRAM OF 2-DIMENSIONAL PLANE DISPERSION MODEL 3-1

TABLE 3-1

ADVECTION-DISPERSION EQUATION WITH BOUNDARY CONDITIONS AND CLEARY AND UNGS ANALYTICAL SOLUTION

TWO DIMENSIONAL ADVECTION-DISPERSION EQUATION: $\begin{array}{lll} D_L & (\delta^2 C/\delta x^2) + D_T (\delta C^2/\delta y^2) - v(\delta C/\delta x) - (\text{lambda}) \, (R) \, (C) = \\ R & \delta C/\delta t \\ \text{where,} & \\ D_L & = \text{longitudinal dispersion, in } L^2/T \\ D_T & = \text{transverse dispersion, in } L^2/T \\ v & = \text{seepage velocity, in } L/T, \\ \text{lambda} & = \text{radioactive decay constant, which is zero for the} \end{array}$

Somers site

R = retardation factor for the given type of solute
t = time, L

INITIAL AND BOUNDARY CONDITIONS OF MATHEMATICAL MODEL:

$$C(0,y,t) = C_0e^{-\tilde{a}t}$$
 $-a \le y \le a$
 $C(0,y,t) = 0$ other values of y
 $C(x,y,0) = 0$ where $x > 0$
where,
 C_0 = initial concentration of the solute, in ppm,
 \tilde{a} = decay of solute, in T^{-1}

ANALYTICAL MODEL AS PRESENTED BY CLEARY AND UNGS (1978):

$$C(x, y, t) = \frac{C_0 x}{4(\pi D_x)^{1/2}} \exp\left(\frac{v_x x}{2D_x} - \alpha t\right)$$

$$\cdot \int_0^{t/R} \exp\left[-\left(\lambda R - \alpha R + \frac{v_x^2}{4D_x}\right)\tau - \frac{x^2}{4D_x \tau}\right] \tau^{-3/2}$$

$$\cdot \left\{ \operatorname{erf}\left[\frac{a - y}{2(D_y \tau)^{1/2}} + \frac{v_y}{2}\left(\frac{\tau}{D_y}\right)^{1/2}\right] + \operatorname{erf}\left[\frac{a + y}{2(D_y \tau)^{1/2}} - \frac{v_y}{2}\left(\frac{\tau}{D_y}\right)^{1/2}\right] \right\} d\tau$$

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culated flow velocities at this site are low enough such that turbulent flow, and a corresponding Reynolds number above 10, is not a problem.

- Flow is unidirectional. This assumption is basically 2. correct for the modeled CERCLA Lagoon area as flow direction does not appear to change significantly during the coarse of the year. However, near the CERCLA Lagoon the direction of flow does bend slightly therefore has an easterly and southeasterly component of flow (according to water table maps constructed for the Remedial Investigation Report, This apparently did not affect the ReTeC, 1987a). model output to any great extent; probably because the X axis of the model grid was intentionally oriented such that it is orthogonal to the groundwater gradient and therefore, parallel to the flow direction.
- 3. The porosity is uniform throughout the aquifer. This assumption is not strictly correct for the Somers site. Due to the various lithologies present, the effective porosity could be expected to range from 15 to 50 %, therefore, an average value of 0.3 was chosen to model the "average" extent and rate of migration.
- 4. The hydraulic conductivity is uniform and constant with time. This is probably not an unreasonable assumption for the CERCLA Lagoon area in a horizontal plane since the four measured values of hydraulic conductivity are all quite close in value. In three dimensions, however, this is not the case because of the known variations in lithologies at differing depths.
- 5. Fluid density gradients, viscosity gradients, and temperature gradients do not affect the migration of

the modeled contaminants. This is not entirely true at this site because creosote is a dense NAPL and will migrate downward in the subsurface under the influence of gravity. A number of borings have been drilled in the CERCIA Lagoon and have delineated the extent of creosote NAPL to depths of approximately 50 feet in areas where liquid creosote was known to have collected in pools at the surface. The greatest extent of any plume migration, however, would be caused by transport of naphthalene as a solute and not as a free product NAPL.

- 6. Molecular diffusion is a negligible component of the total dispersion. This would be true in a groundwater system such as exists in the CERCLA Lagoon area where the pore water velocity is 34.7 m/sec.
- 7. The aquifer is homogeneous and isotropic. This is almost never the case due to the variations in site In the CERCLA Lagoon area, beds of silts, clays, and fine-grained sands are interbedded within the deltaic sand aquifer. The parameters chosen to represent the aquifer characteristics for the model were therefore varied to take into consideration the nonhomogeneity of the aquifer. The aquifer is also not considered to be isotropic. According to Todd (1980), ratios of horizontal to vertical permeability can reach values of up to 100 or greater when clay layers are At Somers, the ratio may be somewhat less than 100 because the aquifer rarely contains pure clay This shouldn't adversely affect a twomaterial. dimensional model as long as the modeled aquifer is at the same horizon across the modeled area. In fact, the abundance of clay will help to diminish any vertical flow of groundwater between aquifers and make a two-

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dimensional model more accurate than it would be otherwise.

Other site specific limitations include the fact that the model assumes one-dimensional flow with two-dimensional advection-dispersion. The model does not make any assumptions regarding the vertical flow.

The shallow aquifer was the only one considered to simulate solute transport. At Somers, there exists a small vertically upward flow component (as evidenced in wells 85-la&b, 85-6a&b and 85-8a&b). Transport of solute would therefore have a tendency to remain within the upper aquifer.

The model also assumes that the aquifer is infinite in vertical and horizontal areal extent. With Flathead Lake situated about 1600 feet from the CERCLA Lagoon and the bedrock outcrops to the south, it is evident that the aquifer is not infinite horizontally. In addition, the aquifer is not infinite in the vertical extent either. The modeled aquifer is in fact only about four feet thick and is bounded above and below by a clay aquiclude.

3.3 Data Input

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The analytical solution was coded in Fortran 4 by Berkeley Hydrotechnique, Inc. of Berkeley, California. Software by Microsoft (Version 4.01) was used to compile the code. The program was then run on a personal computer with a math coprocessor. The code stipulates that the input data is entered in an open Fortran format. A copy of the computer code is presented in Appendix A. For the CERCLA Lagoon, the input data was entered into an input file consisting of seven lines of data as described below:

First line of input data:

numx = number of x coordinates at which concentration of the solute is calculated. Generally, the interval between x-coordinates increases with increasing distance from the source.

numy = number of y coordinates at which the concentration for the solute is calculated. The interval between y-coordinates also increases with increasing distance from the source.

numt = number of time steps at which model is run.

Second line of input data:

X coordinates at which solute concentrations will be calculated. The number of x-coordinates was provided in line 1 of input data file.

Third line of input data:

Y coordinates at which solute concentrations will be calculated. The number of y-coordinates was provided in line 1 of input data file.

Fourth line of input data:

The number of time steps at which solute concentrations are calculated.

Fifth line of input data:

DL = longitudinal dispersion term

DT = transverse dispersion term

V = pore water velocity or seepage velocity

A = half length of strip source (see Figure 3-1)

Sixth line of input data:

alam = decay constant of the solute

R = retardation factor

ã = decay constant of the source

Seventh line of input data:

Co = initial concentration of solute in groundwater along the

entire length of the strip source.

The input are entered in metric units and are converted in the program to English (or traditional) units. The specific input data used for the CERCLA Lagoon model runs will be discussed in Section 3.4.

The first page of the computer model output repeats the input data file with the values listed for each parameter in metric units. The rest of the output file contains a list of the x-coordinate values (in feet), the y-coordinate values (in feet), and the concentration of the solute (in parts per million).

Verification of the analytical solution is provided in Javendal et. al. (1984) so that users of the solution can verify that their code solves the equations accurately. For instance, tables of results are provided by Cleary and Ungs containing set input parameters, including time, velocity, half-length of source, longitudinal dispersion coefficient, transverse dispersion coefficient, retardation factor, decay factor of source, and decay factor of solute. The output in the verification table is provided as C/C_0 . Table 3-2 provides a list of the input parameters used to verify the analytical model and computer code used for the Somers site. The output concentrations are also provided and compared to values generated by the authors of the solution to verify the results.

3.4 Parameter Values

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A description of the input parameter values chosen for the CERCLA Lagoon analytical model is provided in the following subsections. The parameters are described in the order in which they are entered in the input file. Most of the parameters were varied to determine their sensitivity, to calibrate the model, and to allow for variation of values representing aquifer characteristics.

The compound chosen for solute transport modeling was

Table 3-2 VERIFICATION OF ANALYTICAL CODE

	VERIFICATION INPUT PARAMETERS											
nuax = 9	numy = 6	numt = 1										
x = 10	x = 15	x = 20	x = 25	x = 30	x = 35	x = 40	x = 45	x = 50				
y = 5	y = 10	y = 20	y = 30	y = 40								
t = 100												
D(l) = 1	D(t) = 0.1	v = 0.1	A = 50									
alsa = 0	r = 1	alpha = 0										
coni = 1												
					VER I	FICATION OU	TPUT					

	Y = 0		' * O Y = 5		Y =	Y = 10		Y 20		30	Y = 40	
X VALUES	MODEL CONC	AUTHOR CONC	MODEL CONC	AUTHOR CONC	MODEL. CONC	AUTHOR CONC	MODEL. CONC	AUTHOR CONC	MODEL CONC	AUTHOR CONC	MODEL	AUTHOR CONC
10.00049	0.71379	0.71379	0.71379	0.71379	0.71379	0.71379	0.71379	0.71379	0.71379	0.71379	0.71271	0.7127
15.00073	0.53461	0.53461	0.53461	0.53461	0.53461	0.53461	0.53461	0.53461	0.53461	0.53461	0.53322	0.5332
20.00098	0.36498	0.36498	0.36498	0.36498	0.36498	0.36498	0.36498	0.36498	0.36498	0.36498	0.36361	0.3636
25.00122	0.22561	0.22561	0.22561	0.22561	0.22561	0.22561	0.22561	0.22561	0.22561	0.22561	0.22451	0.2245
30.00146	0.12563	0.12563	0.12563	0.12563	0.12563	0.12563	0.12563	0.12563	0.12563	D. 12563	0.12489	0.12489
35.00323	0.06277	0.06277	0.06277	0.06277	0.06277	0.06277	0.06277	0.06277	0.06277	0.06277	0.06234	0.06234
40.00195	0.02806	0.02806	0.02806	0.02806	0.02806	0.02806	0.02806	0.02806	0.02806	0.02806	0.02784	0.0278
45.00372	0.01119	0.01119	0.01119	0.01119	0.01119	0.01119	0.01119	0.01119	0.01119	0.01119	0.01110	0.01110
50.00244	0.00398	0.00398	0.00398	0.00398	0.00398	0.00398	0.00398	0.00398	0.00398	0.00398	0.00394	0.00394

naphthalene. While several other PAH constituents have been detected in groundwater, a review of these compounds showed that naphthalene was more mobile in groundwater since it has a greater water solubility and a lower octanol/water partition coefficient. Other PAH compounds more strongly sorb to soil particles and are less mobile than naphthalene, therefore, naphthalene represents the most conservative PAH constituent to model.

3.4.1 X-Coordinate Values

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The x-coordinate values are chosen by first estimating their values and running the model to determine the distance the solute travels from the source. The values can then be refined to ensure that the output values are bounded within the x-coordinate grid.

For some of the model runs, it was necessary to substantially alter the x-coordinate values. This was especially true for cases when the hydraulic conductivity was increased or the retardation factor was decreased. The highest x-value input into the model was about 5,000 meters (16,400 feet) for run #6 when the retardation factor was decreased to 1 (no retardation). The x-coordinate values are entered in meters.

3.4.2 Y-Coordinate Values

The y-coordinate values are chosen based on the length, 2A, of the source. The total length of the CERCLA Lagoon was estimated to be 200 feet based on areal photographs and visual inspection. Therefore, the y-coordinate values should range from 0 to at least 100 feet (30.5 meters). Only one-half of the y-coordinate values are input since the program assumes that the values entered in the positive y-direction are the same values in the negative y-direction. The greatest y-coordinate value was chosen to be 164 feet (50 meters).

3.4.3 Time Steps

The Remedial Investigation Report (ReTeC, 1987a) describes the history of waste disposal at the site with the earliest record showing a waste sump near the present day CERCLA Lagoon. This record was dated 1927. Based on this information, an assumption was made that 1927 was the earliest possible date groundwater could have been contaminated with creosote.

The majority of model runs were run with two time steps; the first at 60 years and the second at 120 years. Assuming that groundwater contamination first occurred in 1927, the first time step was run for 60 years to bring the model to essentially the present day. A second time step of 120 years was chosen to predict solute transport 60 years into the future which would be Later time steps were not run because the model the year 2047. must be further calibrated with more groundwater quality data before it is known whether or not it is able to accurately predict naphthalene transport over time down-gradient from the CERCLA Lagoon. If the model proves to be accurate, then additional model runs further out into the future can be considered.

3.4.4 Velocity, Hydraulic Conductivity, and Gradient

Velocity as used in the advection-dispersion equation is the average pore water velocity as defined by the equation:

 $v_s = Ki/n$

where,

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K = hydraulic conductivity (in cm/s)

i = hydraulic gradient

n = effective porosity.

Hydraulic conductivity was determined by actual field measurements. The information from several slug tests was used to calculate an average value for the hydraulic conductivity which is 3.3×10^{-3} cm/sec (Table 2-1). Additionally, the model was run with values for the hydraulic conductivity two orders of magnitude above and below this average value in order to ascer-

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tain the sensitivity of the model to changes in this parameter. In all, five model runs were modeled using differing values of hydraulic conductivity.

The hydraulic gradient (i) was measured as 0.01 ft/ft in the area of the CERCLA Lagoon. Groundwater contour maps included in the Remedial Investigation (ReTec, 1987a) were used to arrive at this value.

The effective porosity (n) was arrived at by assuming a typical value of 0.3, which is usually used in most modeling attempts because field measured values are difficult, expensive, and can take up to a year to acquire.

Based on the average value for hydraulic conductivity of 3.3 \times 10⁻³ cm/sec, a gradient of 0.01, and an effective porosity of 0.3, the average pore water velocity was calculated as 34.7 m/year.

3.4.5 Longitudinal Dispersion Term

Dispersion is a result of two processes, molecular diffusion and mechanical mixing. It causes solute to spread over a greater volume of aquifer and is affected by vertical and horizontal conductivity and the degree of stratification within the aquifer. Longitudinal dispersion is the spreading of the solute in the direction of bulk flow (Freeze and Cherry, 1979). Longitudinal dispersion values may be approximated by conducting a column test on a sample of material in the laboratory and determining the breakthrough curve for the solute. Dispersion coefficients can be found from tracer tests in the field. Dispersion coefficients can also be estimated from the equation:

 $D_{L} = (\tilde{a}_{L})(V_{S}) + D^{*}$

where,

 D_{T} = coefficient of longitudinal dispersion

 \tilde{a}_L = dynamic dispersivity (a characteristic of the porous medium).

 v_s = seepage velocity or average pore water velocity

D* = coefficient of molecular diffusion.

The product of the dynamic dispersivity and the average pore water velocity is referred to as the coefficient of mechanical dispersion. According to Anderson (1984), the coefficient of mechanical dispersion is usually a few orders of magnitude larger than the coefficient of molecular diffusion. In most practical applications, therefore, the effects of molecular diffusion can be neglected.

For the CERCLA Lagoon at Somers, \tilde{a}_L is approximated using a distribution chart of dynamic dispersivity values for porous and fractured media (Javendal et al 1984). According to these charts, an average value for dynamic dispersivity is 5 meters. For silts and clays, this value is somewhat high and is therefore a conservative estimate.

For most of the model runs, a value of 5 meters was used for this parameter. Dynamic dispersivity was however, varied from 1 to 20 meters to test the sensitivity of the model to this parameter.

The value for dynamic dispersivity was multiplied by the calculated value for velocity to derive the coefficient of longitudinal dispersion. For example, using a velocity of 34.7 m/year and a dynamic dispersivity of 5 meters resulted in a value of 173.45 m²/year for the longitudinal dispersion.

In every model run where the value for hydraulic conductivity was changed, new values for velocity and dispersion had to be calculated.

3.4.6 Transverse Dispersion Term

In general, the $D_{\rm T}$ term is considered to be one order of magnitude less than the $D_{\rm L}$ term (Javendal et al, 1984). Therefore, when $D_{\rm L}$ = 173.45 m²/year, DT would be 17.34 m²/year.

3.4.7 Half Length of Strip Source

The length of the CERCLA Lagoon was determined in the field

to be about 200 feet, therefore the half-length is 100 feet or 30 meters. For a few model runs however, a strip source half-length of 50 feet or 15 meters was used solely to observe how the resulting plume would look.

3.4.8 Decay Factor of Solute

Biological or chemical degradation of the solute is taken into consideration with the decay term. While some research has been done to arrive at values of biological degradation of PAH constituents dissolved in groundwater, values are still considered to be experimental. Therefore, for most of the model runs a value of zero (no degradation) was used to model the most conservative situation.

However, relatively high rates of biodegradation of PAH in soil/water systems have been documented in numerous studies. example, Mihelcic and Luthy (1988a & 1988b) found half-lives for naphthalene degradation of 3 days under aerobic conditions and 23 days under denitrification conditions. Unfortunately, little detailed information exists on degradation mechanisms and rates for PAH compounds in groundwater systems. Borden et. al. (1984) did find that PAH's in a contaminant plume from an abandoned creosoting site were undergoing biodegradation; however, the rate of degradation was limited by the availability of oxygen. authors estimated the degradation rate at 0.365/year, which corresponds to a half-life of about 2 years. When their model was actually applied in the field it was found that accurate results could be obtained only when the degradation rate was set to "unrealistically low values" of 0.0365/year (half-life = 19 vears).

In a number of model runs, this parameter was varied from a range of 84.32/year (half-life = 3 days) to 0.231/year (half-life = 3 years). In this way, the sensitivity could be determined of the model to this parameter.

3.4.9 Retardation Factor

The retardation factor represents the advancing front of sorbing solute which moves at a linear velocity smaller than the velocity of groundwater movement. The retardation factor is based on the equation (Roberts, 1987):

 $R = 1 + (\delta_b \times K_d)/n$

where,

R = retardation factor

bulk density of material

which the solute flows in g/m3 K_d = distribution coefficient in m^3/g

= porosity.

The bulk density of the matrix through which the solute flows is estimated from the equation (Roberts, 1987):

 $\delta_b = (1 - n) \times \delta_S + n \times \delta_W$

where,

n = porosity, 0.3

 δ_s = density of soil, 2.65 x 10⁶ g/m³ δ_w = density of water, 1 x 10⁶ g/m³.

Therefore, δ_b is estimated to be 2.2 x 10^6 g/m³.

The distribution coefficient (Kd) is used to represent the partitioning of a contaminant between the solution phase and the solid phase. Different methods have been used to determine the distribution coefficients of different contaminants. One method involves the use of laboratory column leach experiments where effluent concentrations are measured in order to determine the partitioning between the liquid phase and the solid matrix. Another method involves the measurement in the field of contaminant concentrations in the soil samples collected at various depths during drilling and in adjacent groundwater during subsequent monitoring well sampling. The third and most widely used method involves the calculation of Kd based on the total organic carbon content of the soil. This is the method that was chosen for this site.

It has been shown that the greater the organic carbon

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content of the soil the greater the solute will sorb onto the material (Roberts, 1987). The following equation illustrates the correlation:

 $K_{d} = 6.3 \times 10^{-7} \times f_{oc} \times K_{ow}$ where,

K_{OW} = octanol/water partition
coefficient.

Log K_{OW} values for naphthalene range in the literature but are typically about 3.32 (Hansch and Leo, 1979). The K_{OW} value is thus 2089. The organic carbon content in the soils from borings #88-1, #88-2, and #88-3 was found to be 1.6 percent. Using this value in the equation above, K_{cd} becomes 2.11 x 10^{-5} m³/g. Combining the value of K_{cd} with the bulk density term of 2.2 x 10^{6} results in a retardation factor (R) of 156.

This value for retardation, when applied to the actual field data, was found to retard naphthalene transport to a much greater extent than was actually the case. Therefore, numerous model runs were constructed varying the retardation from a high of 156 to a low of 1 (no retardation). This provided information on the sensitivity of the model to this parameter as well as being used to calibrate the model to the actual field data.

3.4.10 Decay Factor of the Source

A value of zero was entered for this parameter at the Somers site. Field evidence indicates that within the CERCLA Lagoon free product creosote exists. It seems apparent that even after 60 years duration little degradation of the source appears to be taking place. This is probably due to the high concentrations at the source inhibiting the growth of microbial organisms capable of breaking down creosote and its constituents.

3.4.11 Initial Concentration of Solute in Groundwater

The initial concentration of naphthalene in groundwater was chosen to be equal to the solubility of the compound in water (34 mg/L). The dissolved phase is the portion of the waste which has the greatest ability to migrate with groundwater flow and its concentration can be no greater than its solubility. This value was used for most of the model runs and is considered to be the most conservative estimate.

However, in field situations concentrations even close to the solubility of the compound of interest are usually never For instance, MacKay et. al. (1985) has pointed out that organic chemicals are almost never found in groundwater at concentrations even approaching their solubility limits, even when a free product phase is known to exist. Instead, experience has shown observed concentrations to be on the order of 1% to 10% of their solubility limit. An explanation for this is given by MacKay et. al. as being due to diffusional limitations of dissolution and the dilution of the dissolved organic contaminants by dispersion. Therefore, a number of model runs were constructed using Co values between 10 and 1 ppm to determine the sensitivity of the model to this parameter as well as to calibrate some model runs. In addition, one model run was constructed to evaluate the transport of naphthalene assuming enough of the source could be removed such that the initial concentration (Co) in water would be decreased to 1 ppm.

3.4.12 Summary of Model Parameters

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Tables 3-3 through 3-8 present all of the input parameters used in each of the 34 model runs. The tables depict the values used for the x-coordinate grid, y-coordinate grid, time steps, hydraulic conductivities, dynamic dispersivities, degradation of both the source and solute, longitudinal and transverse dispersions, velocities, half length of the strip source, retardation factor, and initial concentration of the solute. Except for the source decay term, all the parameters were varied to obtain

information on the sensitivity of the model to each parameter as well as to aid in fitting the model to the observed field data.

Table 3-3
Input Variables for each Model Run

Parameters	Run 1	Run 2	Run 3	Run 4	Run 5	Run 6
Num(x)	19	32	26	19	19	21
Num(y)	14	17	17	14	14	17
Num(t)	2	2	2	2	2	2
x	(1)	(2)	(3)	(1)	(1)	(4)
Y	**	**	**	**	**	**
T	60,120	60,120	60,120	60,120	60,120	60,120
K	3.30E-03	3.30E-01	3.30E-02	3.30E-04	3.30E-05	3.30E-03
Alfa L	5	5	5	5	5	5
Dl	173.45	17345.00	1734.50	17.34	1.73	173.45
Dt	17.35	1734.50	173.45	1.73	0.17	17.35
V	34.69	3469.00	346.90	3.47	0.35	34.69
A	30	30	30	30	30	30
Alam	0	0	0	0	0	0
R	156	156	156	156	156	1.00
Alfa	0	0	0	0	0	0
Co	34	34	34	34	34	34
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Num(x) = Number of X Coordinates

Num(y) = Number of Y Coordinates

Num(t) = Number of Time Steps

(1) X = X Coordinate Values: 2,5,8,11,14,17,20,23,26,29,32,35,41,

50,60,70,80,90,100 in meters.

(2) X = X Coordinate Values: 10,100,200,300,400,500,600,700,800,900, 1000,1100,1200,1300,1400,1500,1600,1700,

1800,1900,2000,2100,2200,2300,2400,2500,

2600,2700,2800,2900,3000,3100,in meters.

(3) X = X Coordinate Values: 10,50,60,70,80,90,100,120,140,160,180,

200,220,240,260,280,300,320,340,360,380,

400,450,500,550,600 in meters.

(4) X = X Coordinate Values: 10,50,100,150,200,250,300,350,400,450,

500,550,600,650,700,750,800,850,900,950, 1000,1500,2000,2100,2200,2300,2400,2500, 3000,3500,4000,4100,4200,4300,4400,4500,

5000 in meters.

** Y = Y Coordinate Values: 0,2,4,6,8,10,15,20,25,30,35,40,45, 50 in meters.

T = Time Elapsed in years.

K = Hydraulic Conductivity in centimete per second.

Alfa L = Dispersivity in meters.

Dl = Longitudinal Dispersion in square meters per year.

Dt = Transverse Dispersion in square meters per year.

V = Pore Water Velocity in meters per year.

A = Half length of source strip in meters.

Alam = Decay Factor of the Solute in 1/year

R = Retardation Factor

Alfa = Decay Factor of the Source in 1/year

Co = Initial Concentration of Solute in ppm.

Table 3-4
Input Variables for each Model Run

Parameters	Run 7	Run 8	Run 9	Run 10	Run 11	Run 12
Num(x)	22	21	26	29	43	24
Num(y)	14	14	23	25	25	14
Num(t)	2	2	2	2	9	5
X	(1)	(2)	(3)	(3)	(4)	(6)
Y	**	**	**	**	**	**
7	60,120	60,120	60,120	60,120	(5)	(7)
K	3.30E-03	3.30E-03	3.30E-03	3.30E-03	3.30E-03	3.306-03
Alfa L	1	10	5	5	5	5
Dl	34.69	346.90	173.45	173.45	173.45	173.45
Dt	3.47	34.69	17.35	17.35	17.35	17.35
V	34.69	34.69	34.69	34.69	34.69	34.69
A	30	30	30	30	30	30
Alam	0	0	84	11	11	11
R	156	156	156	156	156	156
Alfa	0	0	0	0	0	0
Co	34	34	34	34	34	34

Notes:

Num(x) = Number of X Coordinates

Num(y) = Number of Y Coordinates

Num(t) = Number of Time Steps

- (1) X = X Coordinate Values: 2,4,6,8,10,12,14,16,18,20,23,26,29,32,35,41, 50,60,70,80,90,100 in meters.
- (2) X = X Coordinate Values: 2,5,8,11,14,17,20,23,26,29,32,35,41, 50,60,70,80,90,100,200,400 in meters.
- (3) X = X Coordinate Values: 0.2,0.4,0.6,0.8,1,2,3,4,5,6,7,8,9,10,11,14,17,20 23,26,29,32,35,41,50 in meters.
- (4) X = X Coordinate Values: 1,2,3,4,5,6,7,8,9,10,11,14,17,20,23,26,29, 32,35,41,50,60,70,80 in meters.
- (6) X = X Coordinate Values: 1,2,3,4,5,6,7,8,9,10,11,14,17,20,23,26,29, 32,35,41,50,60,70,80 in meters.
- ** Y = Y Coordinate Values: 0,1,2,3,4,5,6,7,8,10,15,20,25,30,35,40,45,
 50 in meters.
 - T = Time Elapsed in years.
- (5) T = Time Elapsed in years: 0.1,0.2,0.25,0.3,0.4,0.5 in years.
- (7) T = Time Elapsed in years: 1,2,3,4,5 in years.
 - K = Hydraulic Conductivity in centimeters per second.
 - Alfa L = Dispersivity in meters.
 - DI = Longitudinal Dispersion in square meters per year.
 - Dt = Transverse Dispersion in square meters per year.
 - V = Pore Water Velocity in meters per year.
 - A = Half length of source strip in meters.
 - Alam = Decay Factor of the Solute in 1/year
 - R = Retardation Factor
 - Alfa = Decay Factor of the Source in 1/year
 - Co = Initial Concentration of Solute in ppm.

Table 3-5
Input Variables for each Model Run

Parameters	Run 13	Run 14	Run 15	Run 16	Run 17	Run 18
Num(x)	19	9	21	21	19	19
Num(y)	11	11	14	14	11	11
Num(t)	11	18	1	1	6	6
X	(1)	(1)	(5)	(5)	(1)	(1)
Y	**	* **	**	**	**	**
T	(3)	(4)	60	60	(7)	(7)
K	3.30E-03	3.30E-03	3.30E-03	3.30E-03	3.30E-03	3.30E-03
Alfa L	5	5	15	20	5	5
Dl	173.45	173.45	520.35	693.80	173.45	173.45
Dt	17.35	17.35	52.03	69.38	17.35	17.35
V	34.69	34.69	34.69	34.69	34.69	34.69
A	30	30	30	30	30	30
Alam	11	0.693	0	0	0.346	0.231
R	156	156	156	156	156	156
Alfa	0	0	0	0	0	0
Co	34	34	34	34	34	34

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Num(x) = Number of X Coordinates

Num(y) = Number of Y Coordinates

Num(t) = Number of Time Steps

- (1) X = X Coordinate Values: 1,2,3,4,5,6,7,8,9,10,11,14,17,20,23, 26,29,32,35 in meters.
- (5) X = X Coordinate Values: 2,5,8,11,14,17,20,23,26,29,32,35,41, 50,60,70,80,90,100,200,400 in meters.
- (6) Y = Y Coordinate Values: 0,2,4,6,8,10,15,20,25,30,35,40, 45,50,in meters.

T = Time Elapsed in years.

- (3) T = Time Etapsed in years: 0.08,0.17,0.25,0.33,0.42,0.5,0.58,0.67, 0.75,0.83,0.92 in years.
- (4) T = Time Elapsed in years: 0.1,0.2,0.3,0.4,0.5,1,2,3,4,5,6,7,8,9, 10,20,30,40,50,60,120 in years.
- (7) T = Time Elapsed in years: 0.5,1,5,10,60,120 in years.
 - K = Hydraulic Conductivity in centimeters per second.

Alfa L = Dispersivity in meters.

- Di = Longitudinal Dispersion in square meters per year.
- Dt = Transverse Dispersion in square meters per year.
- V = Pore Water Velocity in meters per year.
- A = Half length of source strip in meters.
- Alam = Decay Factor of the Solute in 1/year
- R = Retardation Factor
- Alfa = Decay Factor of the Source in 1/year
- Co = Initial Concentration of Solute in ppm.

Table 3-6 Input Variables for each Model Run

Parameters	Run 19	Run 20	Run 21	Run 22	Run 23	Run 24
Num(x)	19	19	19	21	29	29
Num(y)	14	14	14	14	14	14
Num(t)	2	2	2	1	1	1
x	(1)	(1)	(1)	(3)	(4)	(4)
Y	**	**	**	**	**	**
T	60,120	60,120	60,120	60	60	60
K	3.30E-03	3.30E-03	3.30E-03	3.30E-03	3.30E-03	3.30E-03
Alfa L	5	5	5	5	5	5
DL	173.45	173.45	173.45	173.45	173.45	173.45
Dt	17.35	17.35	17.35	17.35	17.35	17.35
V	34.69	34.69	34.69	34.69	34.69	34.69
A	30	30	30	30	30	30
Alam	0	0	0	0	Ú	0
R	125	100	75	50	25	25
Alfa	0	0	0	0	0	0
Co	34	34	34	34	34	34

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Num(x) = Number of X CoordinatesNum(y) = Number of Y Coordinates

Num(t) = Number of Time Steps

(1) X = X Coordinate Values: 2,5,8,11,14,17,20,23,26,29,32,35,41, 50,60,70,80,90,100 in meters.

(3) X = X Coordinate Values: 2,5,8,11,14,17,20,23,26,29,32,35,41, 50,60,70,80,90,100,120,150 in meters.

(4) X = X Coordinate Values: 2,5,8,11,14,17,20,23,26,29,32,35,41, 50,60,70,80,90,100,110,120,130,140,150, 160,170,180,190,200 in meters.

** Y = Y Coordinate Values: 0,2,4,6,8,10,15,20,25,30,35,40, 45,50 in meters.

T = Time Elapsed in years.

K = Hydraulic Conductivity in centimeters per second.

Alfa L = Dispersivity in meters.

Dl = Longitudinal Dispersion in square meters per year.

Dt = Transverse Dispersion in square meters per year.

V = Pore Water Velocity in meters per year.

A = Half length of source strip in meters.

Alam = Decay Factor of the Solute in 1/year

R = Retardation Factor

Alfa = Decay Factor of the Source in 1/year

Co = Initial Concentration of Solute in ppm.

Table 3-7
Input Variables for each Model Run

Parameters	Run 25	Run 26	Run 27	Run 28	Run 29	Run 30
Num(x)	21	21	21	21	21	21
Num(y)	14	14	14	14	14	14
Num(t)	1	1	1	1	1	1
X	(1)	(1)	(1)	(1)	(1)	(1)
Y	**	**	**	**	**	**
T	60	60	60	60	60	60
K	3.30E-03	3.30E-03	3.30E-03	3.30E-03	3.30E-03	3.30E-03
Alfa L	5	5	5	5	5	5
Dŧ	173.45	173.45	173.45	173.45	173.45	173.45
Dt	17.35	17.35	17.35	17.35	17.35	17.35
V	34.69	34.69	34.69	34.69	34.69	34.69
A	30	15	15	15	1	15
Alam	0	0	0	0	0	0
R	35	15	35	35	25	45
Alfa	0	0	0	0	0	0
Co	34	10	10	5	5	10

Notes:

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Num(x) = Number of X Coordinates

Num(y) = Number of Y Coordinates

Num(t) = Number of Time Steps

(1) X = X Coordinate Values: 2,5,8,11,14,17,20,23,26,29,32,35,41, 50,60,70,80,90,100 in meters.

** Y = Y Coordinate Values: 0,2,4,6,8,10,15,20,25,30,35,40, 45,50 in meters.

T = Time Elapsed in years.

K = Hydraulic Conductivity in centimeters per second.

Alfa L = Dispersivity in meters.

Dl = Longitudinal Dispersion in square meters per year.

Dt = Transverse Dispersion in square meters per year.

V = Pore Water Velocity in meters per year.

A = Half length of source strip in meters.

Alam = Decay Factor of the Solute in 1/year

R = Retardation Factor

Alfa = Decay Factor of the Source in 1/year

Co = Initial Concentration of Solute in ppm.

Table 3-8 Input Variables for each Model Run

Parameters	Run 31	Run 32	Run 33	Run 34
Num(x)	29	29	29	21
Num(y)	14	14	14	14
Num(t)	1	1	1	2
x	(1)	(1)	(1)	(3)
Y	**	. **	**	**
T	60	60	60	60,120
K	3.30E-03	3.30E-03	3.30E-03	3.30E-03
Alfa L	5	5	5	5
Dl	173.45	173.45	173.45	173.45
Dt	17.35	17.35	17.35	17.35
V	34.69	34.69	34.69	34.69
A	15	15	15	30
Alam	0	0	0	G
R	25	30	25	35
Alfa	0	0	0	0
Co	10	10	5	1

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Notes: Num(x) = Number of X Coordinates

Num(y) = Number of Y Coordinates

Num(t) = Number of Time Steps

(1) X = X Coordinate Values: 2,5,8,11,14,17,20,23,26,29,32,35,41, 50,60,70,80,90,100,110,120,130,140, 150,160,170,180,190,200 in meters.

(3) X = X Coordinate Values: 2,5,8,11,14,17,20,23,26,29,32,35,41, 50,60,70,80,90,100,120,150 in meters.

** Y = Y Coordinate Values: 0,2,4,6,8,10,15,20,25,30,35,40, 45,50 in meters.

T = Time Elapsed in years.

K = Hydraulic Conductivity in centimeters per second.

Alfa L = Dispersivity in meters.

Dl = Longitudinal Dispersion in square meters per year.

Dt = Transverse Dispersion in square meters per year.

V = Pore Water Velocity in meters per year.

A = Half length of source strip in meters.

Alam = Decay Factor of the Solute in 1/year

R = Retardation Factor

Alfa = Decay Factor of the Source in 1/year

Co = Initial Concentration of Solute in ppm.

4.0 MODELING RESULTS

4.1 Model Calibration

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This modeling study addressed the migration of a plume of naphthalene down-gradient from a source located in the CERCLA Lagoon. Figures 4-1 and 4-2 graphically present the results of the first modeling run using what was initially thought to be best estimates for the input parameters. The value used for the hydraulic conductivity was the average value determined from field measurements. The value used for retardation was determined by measuring the organic carbon fraction of the soil in the field and then calculating a value for R. All other parameters are either calculated based on the value of hydraulic conductivity or values reported in the literature are used.

Figure 4-2 shows the plume map generated by this model run. It is evident from this map that the plume is not large enough to encompass all of the contamination actually found in the field. At the 0.1 ppm concentration contour, the plume has only migrated about 150 feet from the source; whereas, Well #88-3 is about 425 feet down-gradient from the source and has a naphthalene concentration of 0.15 ppm. Obviously, the plume is more mobile than the initial input parameters would indicate. In order to better calibrate the model to the actual naphthalene concentrations found in the field, most of the parameters were varied until achieving what was considered a "best fit" between model results and actual field conditions.

Figure 4-3 and Figure 4-4 graphically present the results of what was determined to be the "most realistic" model run for this site. It should be noted that all model results were plotted as C/Co versus distance along the X axis. The X axis distance (Figure 3-1) represents the furthest modeled distance downgradient from the source that the contaminant can migrate. It was felt that a graphical representation of the output was easier to interpret than the raw model output which consisted entirely

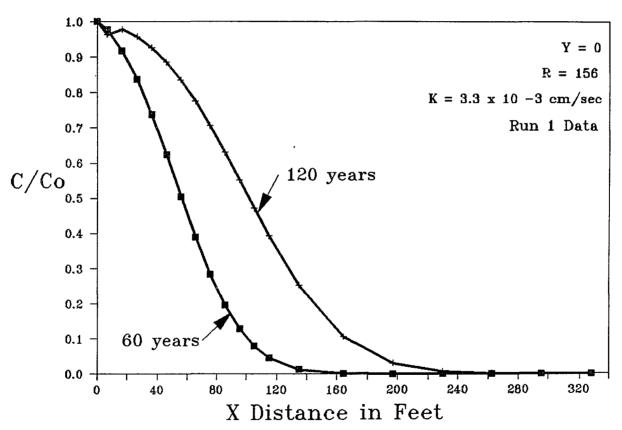


Figure 4-1. Predicted Transport of Naphthalene based on Actual Field Measured Values

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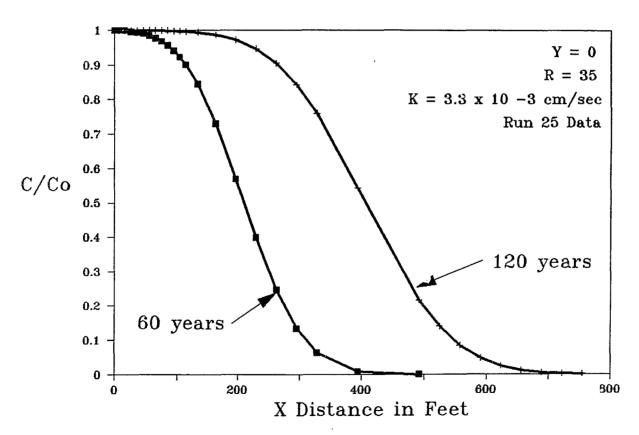


Figure 4-3. Results of Model Run #25, which Provided the Best Fit between the Actual Concentration of Naphthalene and the Predicted Values based on the Model

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of numerous pages of unlabeled columns of numbers. In addition, those model runs which initially appeared to best fit the groundwater quality data, or in some other way were thought to be informative, were also plotted as a plume in plan view on the map. Not all of the model runs were contoured in this manner due to the fact that each of them had to be contoured by hand.

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To obtain the result depicted in Figures 4-3 and 4-4, the model was calibrated by varying the retardation factor from a high of 156 (the calculated value) to a low of 1. In all, eight computer runs were used to calibrate the model to this parameter. Figure 4-5 presents the results of six of the model runs in which retardation was varied from 156 to 15. Figure 4-6 presents the results of a model run in which no retardation (R = 1) was modeled. Obviously, the model is very sensitive to changes in the retardation factor. For instance, at the C/Co = 0.5 point, naphthalene migration is about 70 feet when R = 156 and about 5300 feet when R = 1 after 60 years. This time step corresponds to the present situation found at the site assuming 1927 was the date when groundwater contamination began.

The "best fit" was found when using the input of Run #25 (Table 3-7), in which the retardation was set to equal 35. In this case, the modeled naphthalene plume was depicted as having migrated about 460 feet down-gradient at the 0.1 ppm concentration level after 60 years time (1987). Although this model run best described the maximum extent of plume migration because it agreed with the concentration reported for Well #88-3, the model did not accurately predict the concentrations found in Wells #88-1 and #88-2. Both of these wells had far less naphthalene in them than predicted: 0.48 ppm actual versus 30 ppm predicted for #88-1 and 1.9 ppm actual versus 19 ppm predicted for #88-2. This large discrepancy can be easily accounted for if the initial concentration Co is reduced to what is felt is a more realistic value of between 5 ppm and 10 ppm. This was done in Runs #26

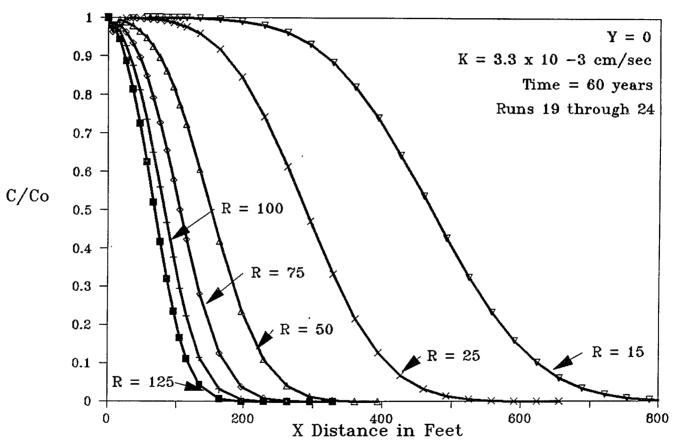


Figure 4-5. Comparison of Naphthalene Transport with Varying Retardation Coefficients

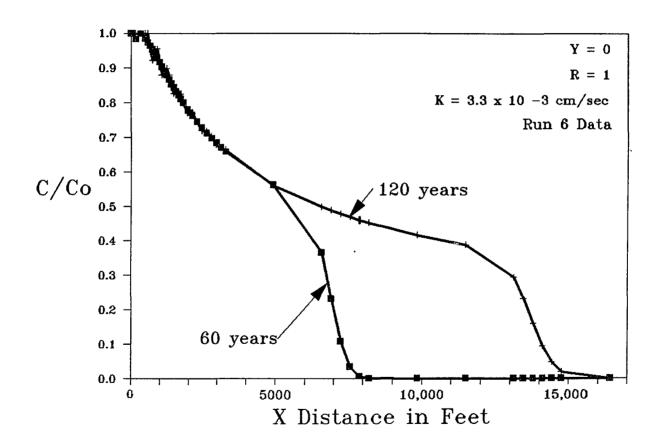


Figure 4-6. Transport of Naphthalene with No Retardation

through #33 (Figures 12 and 13) and the indications are that a very close fit can be achieved for Wells #88-3 and #88-2; however, Well #88-1 would still have a concentration lower than predicted: 0.48 ppm actual versus about 5 ppm predicted. By lowering the initial concentration of naphthalene, the extent of the down-gradient plume at the 0.1 ppm concentration level remains about 460 feet after 60 years time, which is the same result as when Co was set to 34 ppm. The actual naphthalene concentration from Well #88-2 would however, match its predicted value. In addition, the result for Well #88-1 would also be in much closer agreement with its predicted value.

A possible explanation for the difference in calculated versus modeled retardation values could be the existence of inhomogeneities in the distribution of organic carbon throughout the soil profile. If the retardation value is set equal to 35, then the organic carbon fraction value would calculate out to be about 0.0035, which is much less than the measured value of 0.016. However, the measured value might not represent the actual amount of organic carbon present in the aquifer.

Alternatively, the octanol/water partition coefficient of 2089 may be in error or the empirical formula itself might be inaccurate.

4.2 Sensitivity to Hydraulic Conductivity

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The model also proved to be highly sensitive to other variables in addition to the retardation factor. The model in fact, proved to be more sensitive to changes in hydraulic conductivity (K) than any other parameter. This result was anticipated due to hydraulic conductivity being used to calculate many of the other variables input into this model. Many of the other parameters are therefore not independent variables, and are instead dependent on the value for hydraulic conductivity.

Figure 4-7 depicts the transport of naphthalene with successive one order of magnitude changes in the hydraulic

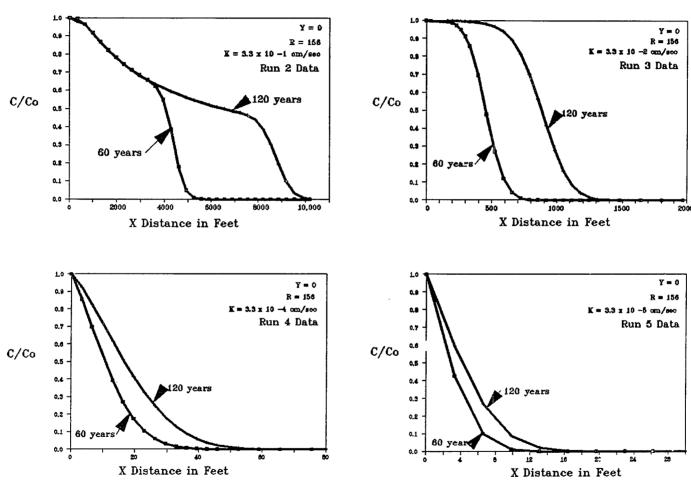


Figure 4-7. Comparison of Naphthalene Transport Distances with varying Hydraulic Conductivities

conductivity. Figure 4-2 shows the plume derived with the field measured value of 3.3 x 10⁻³ cm/sec for hydraulic conductivity. Figures 4-8 through 4-11 depict the other plumes that would be generated with changes in K of two orders of magnitude above and below this value. As can be seen in Figure 4-7, naphthalene migration at the C/Co = 0.5 point ranges between a low of 3 feet when $K = 3.3 \times 10^{-1}$ cm/sec to a high of about 4000 feet when $K = 3.3 \times 10^{-5}$ cm/sec at 60 years.

It is apparent that with this range of migration distances, the model could have been calibrated to the groundwater quality data by varying K instead of the retardation. A value of K somewhere between 3.3 x 10^{-3} and 3.3 x 10^{-2} cm/sec would have obtained the desired results. This was not done however, because it was felt that of all the variables input into the model, the hydraulic conductivity was the best known and therefore, should not be changed.

4.3 Sensitivity to Dispersivity

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The majority of model runs were run using a best estimate of dispersivity of 5 meters. This value was obtained using a distribution chart of dynamic dispersivity values for porous and fractured media (Javendal et al 1984). This value was however varied in a number of the runs to determine the sensitivity of the model to this parameter. Figures 4-14 and 4-15 depict the results of modeling four separate runs with dispersivities of 1, 10, 15, and 20 meters. At the C/Co = 0.5 point, naphthalene migration is respectively 42 feet, 63 feet, 68 feet, and 76 feet. Adjustments in this parameter did not affect the shape or movement of the contaminant plume to any great degree.

4.4 Sensitivity to Biodegradation of the Solute

The majority of model runs were run with a zero r_te of decay for naphthalene as a solute. This scenario is obviously the most conservative in that no contaminant is removed by decay.

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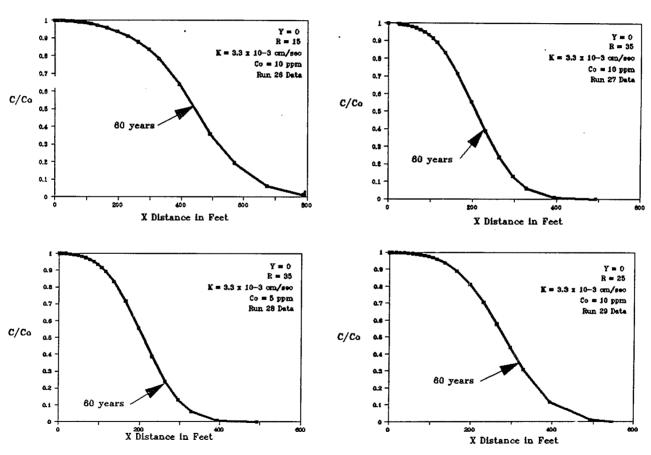


Figure 4-12. Comparison of Naphthalene Transport Distances with Differing Initial Concentrations & Retardation3

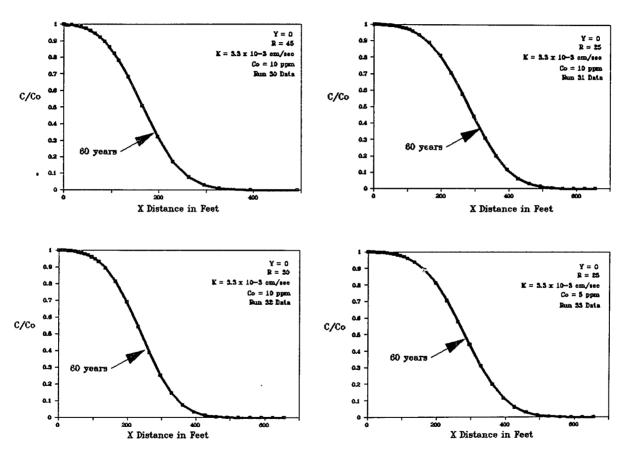
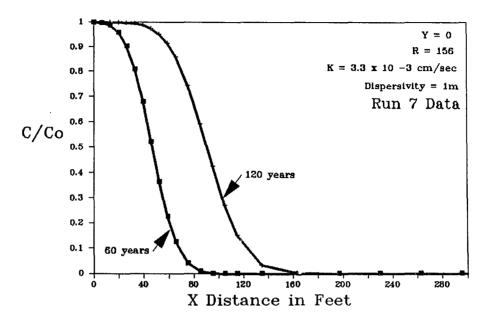


Figure 4-13. Comparison of Naphthalene Transport Distances with Differing Initial Concentrations & Retardations



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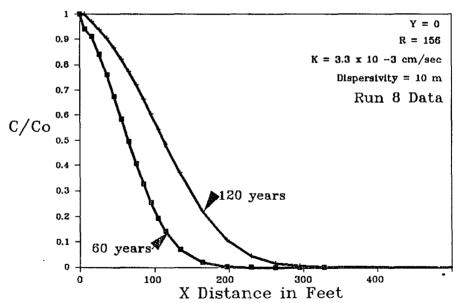
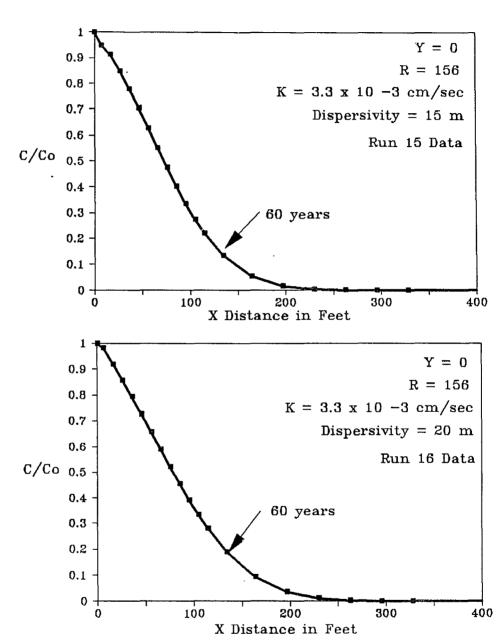


Figure 4-14. Comparison of Naphthalene Transport
Distances with Differing Dispersivities



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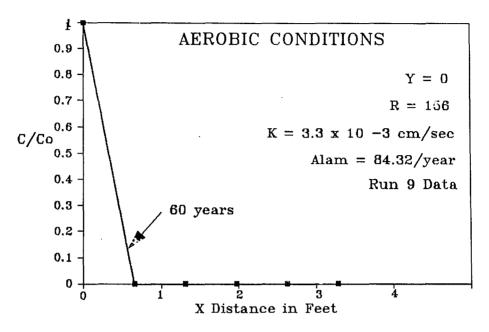
Figure 4-15. Comparison of Naphthalene Transport Distances with Differing Dispersivities

Nevertheless, in order to obtain an understanding of the sensitivity of the model to biodegradation, model runs #9 through #14 (Tables 3-4 and 3-5) were run with varying rates of solute decay. Figures 4-16, 4-17, 4-18, and 4-19 depict the results of some of these modeling runs.

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As discussed in Section 3.4.8, a number of decay rates were chosen from the available literature to simulate degradation under both aerobic and denitrification conditions for both soil/water systems and groundwater systems. Decay rates were input into the model of 84.32/year, 11/year, 0.693/year, 0.346/year, and 0.231/year. These rates correspond to half-lives of 3 days, 23 days, 1 year, 2 years, and 3 years. In addition, numerous time steps were modeled which included inputs of 0.1, 0.2, 0.25, 0.3, 0.4, 0.5, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 20, 30, 40, 50, 60, and 120 years.

The model proved to be very sensitive to this parameter in that no matter what the rate of decay input into the model or the time steps chosen, migration of contaminant was limited to within a few feet of the source. For instance, Figure 4-16 compares the transport distances of naphthalene under aerobic and denitrification conditions in soil/water systems and shows that migration is limited to less than 1 foot and about 5 feet in 60 years. Figure 4-17 plots transport distances under denitrification conditions for time intervals between 0.1 and 0.5 years. Comparison between these two figures shows essentially difference between migration distances, no matter what time interval is used. Figures 4-18 and 4-19 compare transport distances with varying half-lives of 1, 2, and 3 years for time intervals of 0.5, 1, 5, 10, 60, and 120 years. Only slight increases in transport distances at the 0.1 ppm concentration level were found with increasing half-life values. For instance, at the 0.1 ppm _evel and 60 year time interval, maximum transport distances are about 22, 30 and 38 feet for half-lives of 1, 2, and 3 years.



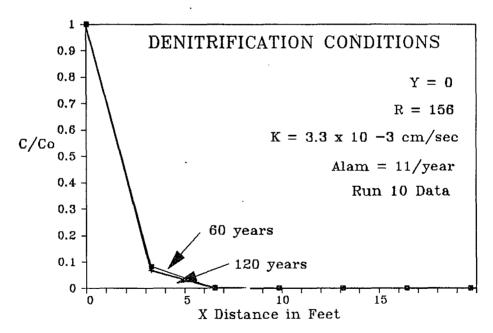


Figure 4-16. Comparison of Naphthalene Transport Distances under Aerobic & Denitrification Degradation

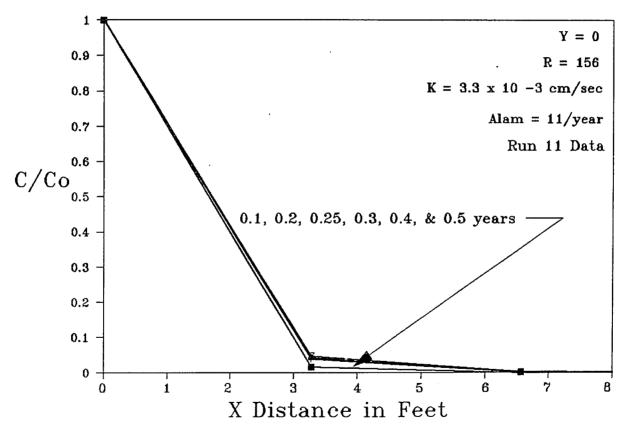


Figure 4-17. Comparison of Naphthalene Transport with Differing Times under Denitrification Conditions

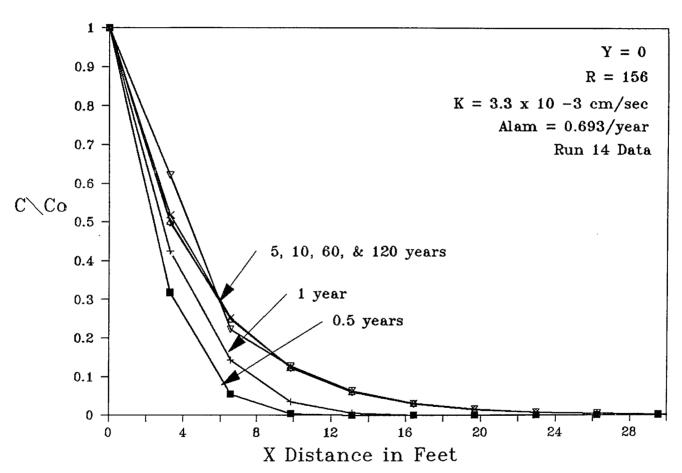
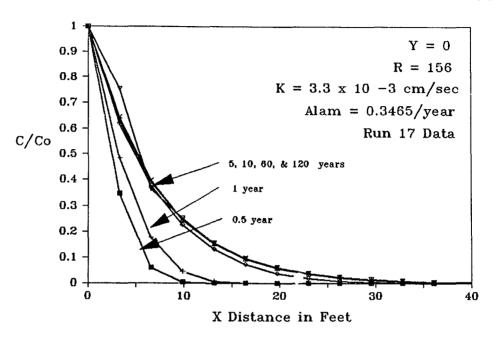


Figure 4-18. Comparison of Naphthalene Transport over Differing Times with a Half-Life of 1 year



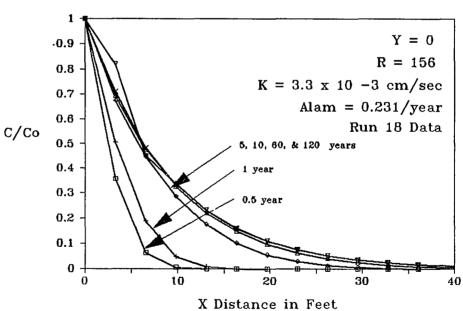


Figure 4-19. Comparison of Naphthalene Transport Distances with Half-Lifes of 2 & 3 years

None of the modeled biodegradation computer runs came even close to predicting the observed extent of naphthalene plume migration. Apparently, very little if any biodegradation of naphthalene appears to be occurring in the groundwater system. This result was unexpected because a number of studies have indicated naphthalene should readily degrade in groundwater, especially considering the length of time available at this site (60 years). Two explanations for this might be that either the oxygen content of the groundwater has been depleted to near zero or no indigenous microbial population exists that is capable of metabolizing naphthalene.

4.5 Hypothetical Source Removal

An attempt was made to predict the extent of plume migration after removing the majority of the source at the CERCLA Lagoon under a hypothetical remedial action. Source removal was assumed to decrease the initial concentration of naphthalene in ground-water to 1 ppm. The resulting plume that was generated after 60 years time is presented in Figure 4-20. A comparison of this figure with Figure 4-3 shows that although the overall concentration of the plume is drastically decreased under the source removal scenario, the maximum extent of plume migration at the 0.1 ppm level after 60 years is still almost 400 feet. Basically no difference in the extent of the plume was found, regardless if the initial concentration was 34 ppm or 1 ppm.

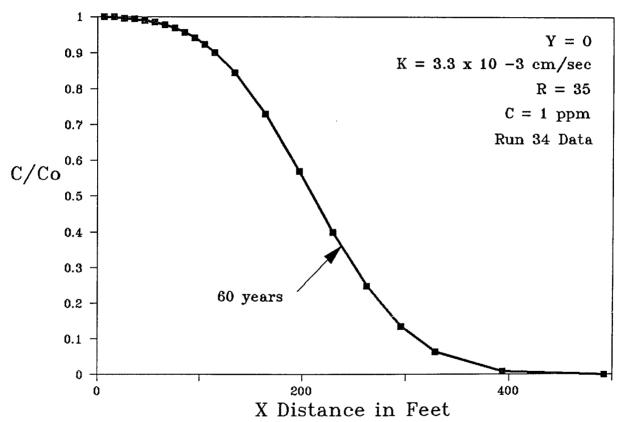


Figure 4-20. Naphthalene Transport Distances after 60 years Assuming Source Removal down to the 1 ppm Level

5.0 SUMMARY AND CONCLUSIONS

The intent of this study was to apply an analytical solutetransport model in the area of the CERCLA Lagoon in an effort to predict the extent of plume migration and naphthalene concentra-Although many assumptions were made in running this model, the modeled results were found to reasonably explain the distribution of the naphthalene plume under varying conditions. It should be noted that this model is a simplification of the actual site conditions and as such, it can not be expected to explain 100% of the variations in contaminant concentrations found at the site. The model can be best used, however, in placing bounds on the problem, testing new ideas, determining which of the parameters are most important in accounting for the majority of variation, and testing clean-up actions. The model also proved to be fairly accurate in determining the maximum extent of plume migration, even though contaminant concentrations at individual wells were often in error.

In summary, a number of conclusions can be made regarding the modeling of naphthalene transport in the vicinity of the CERCLA Lagoon:

- A total of 34 computer runs were modeled in this study.
- 2) The modeling results proved to be extremely sensitive to variations in both the hydraulic conductivity and the retardation coefficient.
- 3) Calibration of the model by varying retardation was chosen as preferable to varying the hydraulic conductivity. The reasoning behind this discission was the value for the average hydraulic conductivity was felt to be better known than the value for the retardation coefficient.
- 4) Calibration of the model was undertaken by varying the retardation a total of eight times from a value of 156 to 1. A retardation of 35 proved to model the maximum extent

of naphthalene migration the best.

- 5) Although the extent of the plume was accurately modeled, naphthalene concentrations at individual wells were found to be much lower than the model predicted.
- 6) Lowering the initial concentration of naphthalene from 34 ppm to between 5 and 10 ppm and keeping the retardation around 35 will give the closest fit between actual data and predicted data.
- 7) The model also proved to be sensitive to variations in degradation rates. Half-lives of 3 days, 23 days, 1 year, 2 years, and 3 years were model as well as numerous time steps of 0.1, 0.2, 0.25, 0.3, 0.4, 0.5, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 20, 30, 40, 50, 60, and 120 years. The results of these modeling runs indicated tha very little plume migration would occur more than a few feet from the source. The maximum extent of plume migration at the 0.1 ppm level was found to be only about 40 feet with a half-life of 3 years and a time interval of 120 years.
- 8) Apparently, very little if any in-situ biodegradation appears to be occurring at this time.
- 9) The model is not sensitive to variations in dispersivity.
- 10) Modeling source removal by assuming the initial concentration of naphthalene in groundwater would be 1 ppm, indicated the maximum extent of the plume would be about the same as when no source removal was undertaken.

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APPENDIX A COMPUTER CODE FOR ANALYTICAL SOLUTION

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                                  3-14-88
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.....
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         include file for strip.for program
        implicit real * 8 (a-h, o-z)
common /ga/ dl, dt, v, a, coni
common /bat/ alfa, alam, r
         common /cat/ xx, yy, tt, tt0
file - strip.for
                               .............
        program test
c test version of code, not commented or cleaned
c from Iraj's agu mono and various numerical methods text
$include:'strip.inc'
         dimension cd(80,80), x(500), y (500), t(20)
         open (5, file='inp')
open (6, file='out')
         read (5,*) numx, numy, numt
if (numx .lt. 1) stop
         read (5,*) (x(i), i=1, numx)
read (5,*) (y(i), i=1, numy)
read (5,*) (t(i), i=1, numt)
read (5,*) dl, dt, v, a
read (5,*) alam, r, alfa
read (5,*) coni
         write (6,610) v, dl, dt, a write (6,620) alem, r, alfa write (6,630) numx, numy, numt write (*,610) v, dl, dt, a write (*,620) alem, r, alfa write (*,630) numx, numy, numt
         do 30 i = 1, numx
do 20 j = 1, numy
                           cd(i,j) = 0.
                  continue
     30 continue
          do 80 it =1, numt
                   tt = t(it) / r
                   do 50 i = 1, numx
                           xx = x(i)
                            do 40 j =1, numy
                                    yy = y(j)
call conc( tt, cd(i,j) )
if (cd(i,j) .le. 1.0d-20) cd(i,j) = 0.0
    40
50
                           continue
                   continue
                  write (6, 640) t(it) write (*, 640) t(it) write (6, 900) format (' x
    900
                                                                         c (ppm)')
                   do 70 iy = 1, numy
```

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do 60 ix = 1, numx
xcord = x(ix) * 3.281d0
ycord = y(iy) * 3.281d0
if (ycord .lt. 1.d-2) then
                                                  write (6,660) xcord, ycord, cd(ix,iy)
                                                  yycord * -ycord
write (6,660) xcord, ycord, cd(ix,iy)
write (6,660) xcord, yycord, cd(ix,iy)
                                         endif
    60
                              continue
    70
                   continue
           continue
  610 format (' v = ', 1pe12.4, 1x, ' dl = ', 1pe12.4, 1x, s ' dt = ', 1pe12.4, 1x, ' a = ', 1pe12.4)
620 format (' alam = ', 1pe12.4, 1x, 'r = ', 1pe12.4, 1x, s 'alfa = ', 1pe12.4)
630 format (' numx = ', i5, 1x, 'numy = ', i5, 1x, 'numt = ', i5)
640 format (' time = ', 1pe12.4)
660 format (3x, 1pe12.4, 3x, 1pe12.4, 3x, 1pe12.4)
         stop
         end
         subroutine func (x5,xsol)
Sinclude: 'anal.inc'
         real*8 derf
pi = 3.14159265d0
          WW = (V^*xx/(2.d0*dl)) - (alfa*tt)
          W = dexp (WW)
          aa = - (alam*r - alfa*r +
$ (v**2)/(4.d0*dl))*x5 - (xx**2/(4.d0*dl*x5))
aaa = dexp (aa)/ dsqrt(x5**3)
          bb = (a-yy)/(2.d0 * dsqrt (dt*x5))
cc = (-a-yy)/(2.d0 * dsqrt (dt*x5))
          bbb = 1.d0 - derf(bb) ccc = 1.d0 - derf (cc)
          pi = 3.14159265d0
          xsol = coni * asa * (ccc -bbb) * (xx/( 4.d0 * dsqrt (pi*dl))) *ww
          return
          end
          real*8 function derf (xz)
           implicit real *8 (a-h, o-z)
          dimension d(101)
          if (dabs(xz) .gt. 3.6d0) then derf = dsign (1.d0,xz)
                     return
          end if
          n = 100
          n1 = n+1
          pi = 3.14159265d0
          c = 2.d0 / dsqrt (pi)
          h = xz/n
           do 130 i = 1, n1
```

```
y = (i-1)*h
                d(i) = dexp(-y^ay)
   130 continue
        e1 = 0.d0
        do 140 i =3, n1, 2
e1 = e1 + (d(i-2) + 4.d0 * d(i-1) + d(i)) * (h/3.d0)
   140 continue
        derf = c * e1
        return
        end
file - strip2.for
       subroutine conc(tt, xxsol)
implicit real=8 (a-h, o-z)
parameter (npoint=30, x1=0.d0, x2=1.d0)
dimension xg(npoint), wg(npoint)
       x3 = tt
       call gauleg(x1, x2, xg, wg, npoint) call gauleg(x1, x3, xg, wg, npoint)
       xxsol = 0.0d0
       do 12 i = 1,npoint
call func(xg(i), xsol)
xxsol = xxsol + wg(i) * xsol
       return
       end
file - strip3.for
       subroutine gauleg(x1, x2, xg, wg, n) implicit real*8 (a-h, o-z)
       real*8 xg(n), wg(n)
       parameter (eps=3.d-12)
       ഔ(∩+1)/2
       xm=0.5d0*(x2+x1)
xl=0.5d0*(x2-x1)
       do 12 i=1,m
               z=dcos(3.141592654d0*(i-.25d0)/(n+.5d0))
               continue
               p1=1.d0
               p2=0.d0
               do 11 j=1,n
                       p3=p2
                       p2=p1
                       p1=((2.d0+j-1.d0)+z+p2-(j-1.d0)+p3)/j
  11
               continue
               pp=n*(z*p1-p2)/(z*z-1.d0)
z1=z
               z=z1-p1/pp
               if(dabs(z-z1).gt.eps)go to 1
               xg(i)=xm-xl*z
               xg(n+1-i)=xm+xl*z
+g(i)=2.d0*xl/((1.d0-z*z)*pp*pp)
               wg(n+1-i)=wg(i)
      continue
       return
```

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end

```
file inp (sample input file)
7 1 2
10. 15. 20. 25, 30. 35. 40. 23. 26. 29. 32. 35. 41. 50. 60. 70. 80. 90. 100. 0. 2. 4. 6. 8. 10. 15. 20. 25. 30. 35. 40. 45. 50. 100. 365.
          0.1
                   0.1
                              50.
0.
                     Ó.
1.
file - out (result from run of sample input file - inp)
 v = 1.0000E-01 dl = 1.0000E+00 dt = 1.0000E-01 a = 5.0000E+01
 alam = 0.0000E+00 r = 1.0000E+00 alfa = 0.0000E+00
 numx = 7 numy = time = 1.0000E+02
                             1 numt =
      X
3.2810E+01
                                  c (ppm)
                        0.0000E+00
0.0000E+00
0.0000E+00
                                          7.1379E-01
                                          5.3461E-01
3.6498E-01
      4.9215E+01
      6.5620E+01
      8.2025E+01
                        0.0000E+00
                                          2.2561E-01
      9.8430E+01
                        0.0000E+00
                                          1.2563E-01
      1.1484E+02
                        0.0000E+00
                                          6.2769E-02
      1.3124E+02
                        0.0000E+00
                                          2.8057E-02
 time = 3.6500E+02
                        c (ppm)
0.0000E+00 9.5269E-01
0.0000E+00 9.1382E-01
0.0000E+00 8.6420E-01
      x
3.2810E+01
      4.9215E+01
      6.5620E+01
      8.2025E+01
                        0.0000E+00
                                          8.0389E-01
      9.8430E+01
                        0.0000E+00
                                           7.3409E-01
      1.1484E+02
1.3124E+02
                                          6.5687E-01
5.7498E-01
                        0.0000E+00
                        0.0000E+00
file - strip.exe (is the executable file, type "strip" to use program)
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